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IGNITION OF A DROP OF FUEL

by

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13 ABSTRACT

The point of ignition and ignition delay period are determined for a drop of radius R_0 placed in a medium with temperature T_∞ assuming that no combustion of fuel vapors occurs before the moment of ignition, Nu=2, the time of thermal and concentration relaxation is infinitesimal, the Lewis-Semenov criterion is equal to one and that all heat physical quantities are independent of temperature.

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Translated for FSTC by Albert L. Peabody
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NOTICE

III

The basic quantities usually determined during the process of ignition are the point of ignition and the ignition delay period. We will seek these quantities for a drop of radius r_0, placed in a medium with temperature T_∞ under the following assumptions: 1) combustion of fuel vapors does not occur until the moment of ignition (similar to the assumption of O. M. Todes in the unstable theory of thermal ignition); 2) Nu=2, which is generally incorrect, since at the initial moment in time $N_u=\infty$, after which it rapidly approaches its stable value of 2; 3) the times of thermal and concentration reaction are infinitesimal (that is the problem is solved in the quasistable statement); 4) there is similarity between the fields of excess concentration and temperature (i. e., the Lewis-Semenov criterion is equal to one); 5) all heat physical quantities are independent of temperature.

The quantity of heat used to heat the drop is significantly greater than the quantity of heat used for evaporation as long as the drop is far from the point of equilibrium evaporation. Therefore, heating of the drop can be analyzed with some approximation without considering evaporation. Assuming that the temperature of the drop is constant through its radius but variable with time, we produce, considering the assumptions made,

$$\frac{T_1}{T_\infty} = 1 - \left(1 - \frac{T_0}{T_\infty}\right)\exp\left(-\frac{3\kappa t}{r_0^2 c_p \rho}\right).$$

Here T_0 is the initial temperature of the drop, T_1 is the (instantaneous) temperature of the drop, k is the heat conductivity coefficient, c_p and ρ are the heat capacity and density of the drop, t is time. In order to produce the distribution of temperature in space, we shall use the fundamental solution of the stable heat conductivity equation for the spherical case:

$$\frac{T_\infty - T}{T_\infty - T_1} = \frac{r_0}{r}. \qquad 1.2$$

Considering equations (1) and (2), we produce, in the quasistable approximation

$$\frac{T}{T_\infty} = 1 - \frac{r_0}{r}\theta_0 \exp\left(-\frac{3\lambda t}{r_0^2 c_p \rho}\right). \qquad 1.3$$

where

$$\theta_0 = \left(1 - \frac{T_1}{T_\infty}\right).$$

According to the fourth assumption made above

$$\frac{T - T_1}{T_\infty - T_1} = \frac{P_{10} - P_1}{P_{10}}.$$

Here P_1 is the partial pressure of fuel vapors, a function of the coordinates and time, while P_{10} is the partial pressure of the fuel vapors on the surface of the drop, determined by the saturated vapor pressure at temperature T_1. Therefore, the following expression can be produced for the distribution of fuel vapor pressure in space at any moment in time:

$$\frac{P_1}{P} = e^{\frac{H}{RT_\infty}} \frac{r_0}{r} \exp\left\{-\frac{H}{RT_\infty\left[1 - \theta_0 \exp\left(-\frac{3\lambda t}{r_0^2 c_p \rho}\right)\right]}\right\}. \qquad 1.4$$

Here H is the molar heat of evaporation of the fuel, a function of temperature and pressure, P is the total pressure, T_2 is the boiling point of the liquid.

Ignition will occur at the point of the local maximum of the rate of the chemical reaction. In all of the following, we will analyze the second order chemical reaction. Actually, at infinity the temperature is great, but the fuel vapor pressure is insufficient. The level of temperature near the surface of the drop is insufficient. Furthermore, the greatest number of collisions leading to formation of the end products of the chemical reaction will occur with the stoichiometric ratio. Therefore, we can write a system of two equations defining the ignition of evaporating liquid fuel:

$$\frac{\partial W}{\partial r} = 0. \qquad 1.5$$

$$P_1 = \psi P_2. \qquad 1.6$$

where P_2 is the partial pressure of the oxidizer (and inert gases),

ϕ is the stoichiometric coefficient,

the rate of the chemical reaction.

For a second order reaction, we can approximately produce, in place of what (1.5) and (1.6)

$$\frac{1}{P_1}\frac{\partial P_1}{\partial r} + \frac{E}{RT^2}\frac{\partial T}{\partial r} = 0, \qquad 1.7$$

$$\frac{P_1}{P_2} = \frac{\psi}{1+\psi} = \varphi, \qquad 1.8$$

where E is the activation energy of the chemical reaction.

Substituting the distributions of temperature and pressure found earlier into (1.7), we can find the ratio of the radius of ignition to the radius of the drop in the t→0 approximation:

$$\frac{r_1}{r'} = \frac{\varphi E}{RT_\infty}\left(1 - \frac{T_0}{T_\infty}\right). \qquad 1.9$$

Following certain calculations, (1.8) leads us to the expression

$$\frac{H}{RT_2} - \frac{H}{RT_\infty\left[1 - \theta_0\left(1 - \frac{3\kappa t}{r_0^2 c_p \rho}\right)\right]} = \ln \frac{\varphi E\theta_0}{RT_\infty}$$

under the condition that $\frac{E\theta_0}{RT_\infty} >> 2$. From this we can find the ignition delay time.

$$\tau_* = \frac{r_0^2 c_p \rho}{3\kappa}\left[1 - \frac{1}{\theta_0}\left(\frac{1 - \frac{T_2}{T_\infty} + \frac{RT_2}{H}\ln\frac{\varphi E\theta_0}{RT_\infty}}{1 - \frac{RT_2}{H}\ln\frac{\varphi E\theta_0}{RT_\infty}}\right)\right]. \qquad 1.10$$

It follows from (1.10) that as temperature T_∞ is increased, the ignition delay period decreases and as $T_\infty \to \infty$, $\tau_* \to 0$. As the pressure in the system increases, the magnitude decreases, which in turn decreases τ_*. Thus, the relationship with pressure is concealed in the heat of evaporation. Formula (1.10) can be significantly simplified if we assume that

$$\frac{RT_2}{8H}\ln\frac{\varphi E\theta_0}{RT_\infty} \ll 1.$$

Actually, for octane, for example, $T_2 \sim 400°K$, $H \approx 10^6$ cal/mol, $\phi \sim 1$, $E = 20000$ cal/mol. Then where $\phi_0 \sim 1$ and $T_\infty = 1100°K$ we have $\frac{RT_2}{H}\ln\frac{F\vartheta_0}{RT_\infty} = 0.17$ << 1. In this case

$$\tau_* = \frac{r_0^2 c_p \rho}{3\kappa}\frac{T_2 - T_0}{T_\infty - T_0}. \qquad 1.11$$

If we assume T_0=300°K, we find using (1.11) for octane with $2r_0$=0.1 cm, c_p=0.5 cal ·g·deg, ρ=0.8 g/cm^3, k=8.10^{-5} cal/cm·sec·deg τ_*=0.44 sec and r_1/r_0 =6.6 .

We can see from the expressions produced that the ignition delay period depends strongly on droplet size. The dependence on temperature is weaker than that usually observed experimentally, which may be related to the assumption of independence of c_p and k on temperature.

We note that in the quasistable approximate analysis presented above, the results produced are independent of the preexponential factor of the chemical reaction. This is explained by the use of conditions (1.5) and (1.6).

For comparison with the approximate solution produced, the system of equations of diffusion and heat conductivity was numerically calculated in the form

$$\frac{\partial c_1}{\partial t} = D\left(\frac{\partial^2 c_1}{\partial r^2} + \frac{2}{r}\frac{\partial c_1}{\partial r}\right) + k_0 c_1 c_2 e^{-\frac{E}{RT}}$$

$$\frac{\partial T}{\partial t} = a\left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}\right) + q\frac{k_0 c_1 c_2 e^{-\frac{E}{RT}}}{\rho c_p RT}$$

with the initial conditions

$$\left.\begin{aligned} T(r>r_0,\ 0) &= T_\infty \\ c_1(r,\ 0) &= 0 \end{aligned}\right| \qquad 1.13$$

and boundary conditions

$$\left.\begin{aligned} T(\infty, t) &\to T_\infty \\ c_1(\infty, t) &\to 0. \end{aligned}\right|$$

$$T_1 = T_\infty\left[1 - \vartheta_0 \exp\left(-\frac{3kt}{r_0^2 c_p^2}\right)\right]$$

$$c_{10} = \frac{P_0}{RT_1}\exp\left[\frac{H}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\right]. \qquad 1.14$$

Here c_1 is the fuel concentration, c_{10} is the concentration of fuel of the surface of a drop, c_2 is the concentration of oxidizer, k_0 is the preexponential factor, q is the heat value of the fuel.

The following values of dimensional quantities were selected for calculation:

$r_0=10^{-1}$ cm; T_0=300°K; T_2=400°K; T_∞ = 1600°K;

$E=4\cdot10^4 \ \frac{cal}{mol}$; $k_0=10^{10} \ \frac{cm^3}{mol\ sec}$;

$a=D=0.1 \ \frac{cm^2}{sec}$; $k=8\cdot10^{-5} \ \frac{cal}{cm\cdot sec\cdot deg}$;

$$c_p=0.5\ \frac{cal}{g\cdot deg.};\quad c_{p_1}=0.3\ \frac{cal}{g\cdot deg}\ ;\quad p=0.8\ \frac{g}{cm^3}\ ;$$

$$p_.=1.2\cdot 10^{-3}\ \frac{2}{cm^3}\ ;\quad q=7.6\cdot 10^3\ \frac{cal}{g.}\ ;\quad P_o = 1\ atm.$$

Calc[illegible]n was performed by the grids method using the M-20 computer. The calculations showed that the increase in temperature begins at t=1.385 sec at 9 radii from the center of the drop. Then the temperature begins to increase significantly, and the temperature maximum approaches the drop.

If we compare the values of τ_* and r_1 produced with the values calculated according to the approximate formulas (1.9) and (1.11), we produce:

$$\frac{r_1}{r_o} = 10.6$$

$$\tau_* = [illegible]\ sec.$$

The correspondence between approximate and precise calculation must be considered quite satisfactory.